WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 09:26 AM EDT

PDB ID	:	2R4S
Title	:	Crystal structure of the human beta2 adrenoceptor
Authors	:	Rasmussen, S.G.F.; Choi, H.J.; Rosenbaum, D.M.; Kobilka, T.S.; Thian, F.S.; Edwards, P.C.; Burghammer, M.; Ratnala, V.R.; Sanishvili, R.; Fischetti, R.F.; Schertler, G.F.; Weis, W.I.; Kobilka, B.K.
Deposited on	:	2007-08-31
Resolution	:	3.40 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

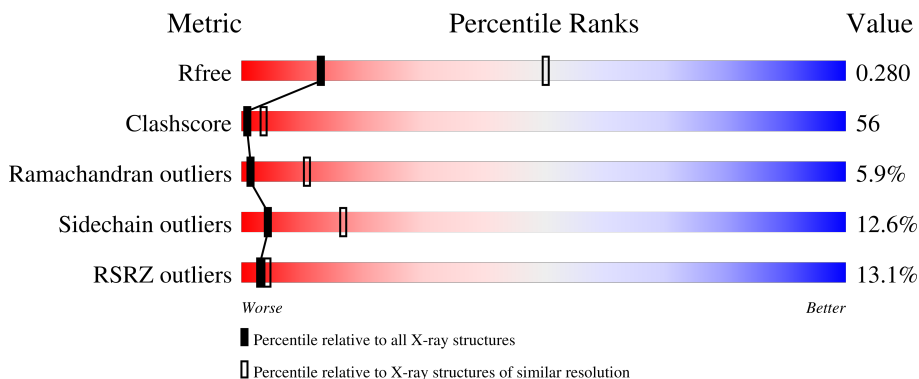|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.280
Clashscore		56
Ramachandran outliers		5.9%
Sidechain outliers		12.6%
RSRZ outliers		13.1%

Worse .... *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	342	22% / 21% 35% 6% • 37%
2	L	214	2% / 29% 57% 12% •
3	H	217	3% / 35% 50% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4925 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-2 adrenergic receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1612	1052	271	279	10			

- Molecule 2 is a protein called antibody for beta2 adrenoceptor, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1678	1050	278	341	9			

- Molecule 3 is a protein called antibody for beta2 adrenoceptor, heavy chain.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1635	1031	269	328	7			

3　Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Beta-2 adrenergic receptor
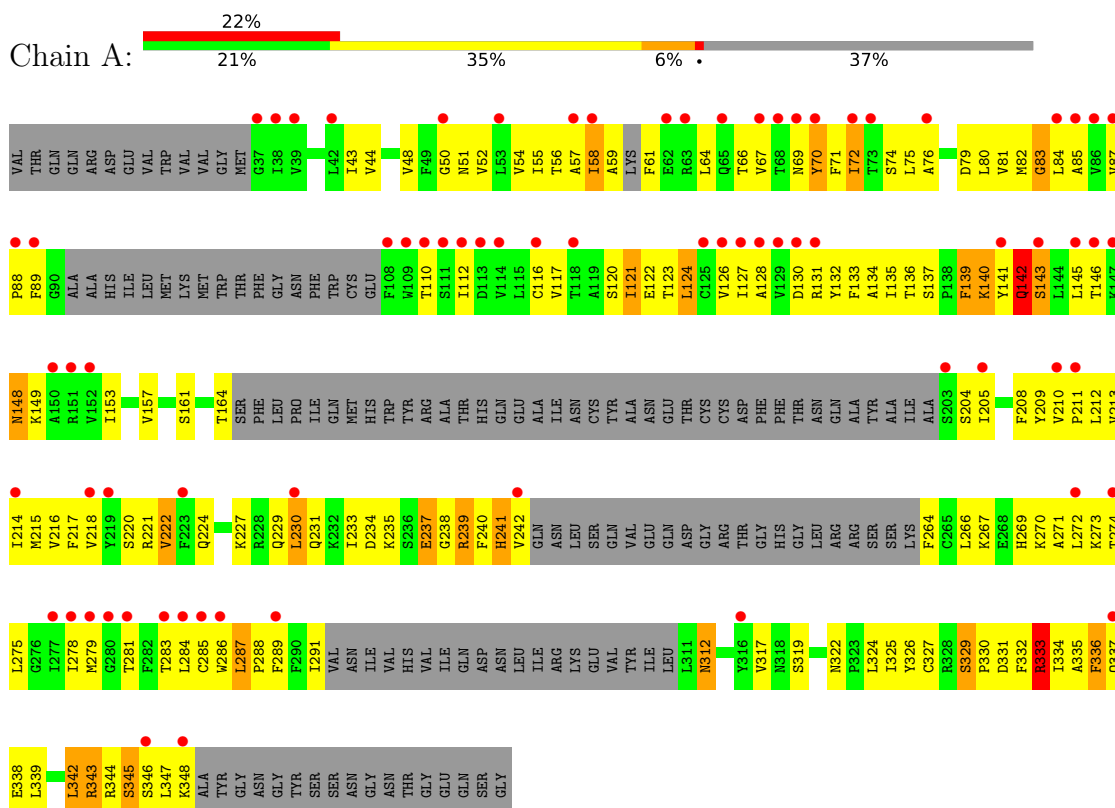
- Molecule 2: antibody for beta2 adrenoceptor, light chain
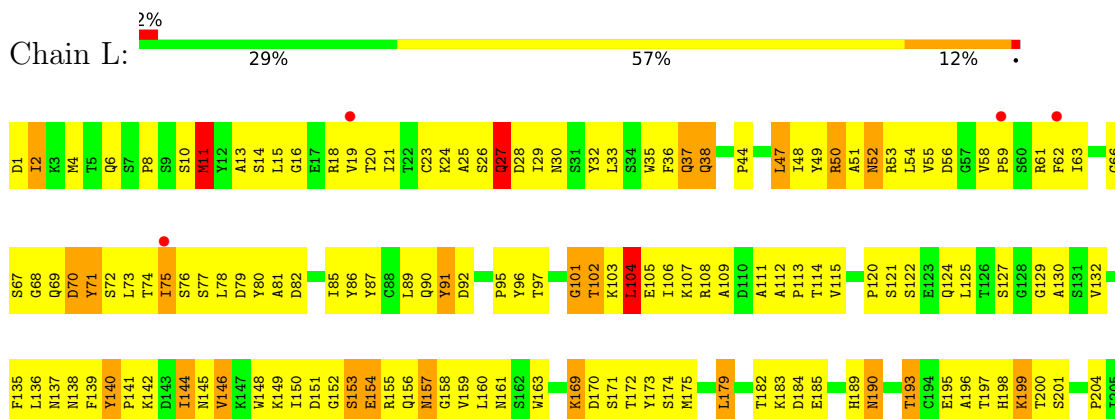
V206 K207 S208 F209 N210 R211 N212 E213 C214

• Molecule 3: antibody for beta2 adrenoceptor, heavy chain

Chain H:

3%

35%　　　　　　50%　　　　　15%

E1 V2 Q3 L4 Q5 Q6 S7 L11 A12 A16 S17 V18 K19 L20 S21 C22 K23 A24 S25 G26 Y27 I28 F29 T30 D31 Y32 Y33 I34 N35 W36 V37 R38 Q39 R40 T41 G42 Q43 G44 F45 E46 W47 I48 I51 Y52 P53 G54 S55 G56 N57 I58 D59 Y60 N61 F64 K67

A68 T69 L70 T71 A72 D73 K74 S77 T78 A79 Y80 M81 Q82 L83 L86 T87 D90 S91 A92 C96 V97 R98 G99 F100 G101 Y102 W103 T107 T108 L109 T110 V111 A114 K115 T116 T117 P118 P119 S120 V121 L124 A125 P126 G127 S128 A129 A130 Q131 T132 N133 S134 A135 V136

T137 L138 G139 C140 L141 V142 K143 G144 Y145 F146 P147 E148 P149 V150 T151 V152 T153 W154 N155 S158 L159 S160 V163 F166 P167 A168 V169 L170 Q171 S172 D173 L174 L177 S178 S179 S180 V181 T182 V183 P184 S185 S186 T187 W188 P189 S190 E191 C195 N196 V197 A198 H199 P200 A201 S202

V206 I210 V211 P212 R213 D214 C215 G216 C217

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	338.38Å 48.48Å 89.35Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	19.99 – 3.40 44.67 – 3.38	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.99-3.40) 96.1 (44.67-3.38)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.226 , 0.280 0.230 , 0.280	Depositor DCC
R_{free} test set	1904 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å^2)	97.9	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 121.7	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.018 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4925	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.35	0/1636	0.56	0/2216
2	L	0.43	0/1716	0.75	1/2324 (0.0%)
3	H	0.44	0/1677	0.75	0/2290
All	All	0.41	0/5029	0.70	1/6830 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	104	LEU	CA-CB-CG	5.54	128.03	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1612	0	1610	184	0
2	L	1678	0	1610	199	0
3	H	1635	0	1578	183	0
All	All	4925	0	4798	549	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 56.

All (549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

W O R L D W I D E
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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:193:THR:HG23	2:L:208:SER:HB2	1.29	1.10
2:L:169:LYS:H	2:L:169:LYS:HD2	1.20	1.03
2:L:108:ARG:HG2	2:L:109:ALA:H	1.25	0.99
2:L:38:GLN:NE2	3:H:39:GLN:HE22	1.60	0.98
2:L:38:GLN:HE21	3:H:39:GLN:HE22	0.98	0.94
3:H:155:ASN:HB3	3:H:158:SER:HB2	1.52	0.90
2:L:38:GLN:HE21	3:H:39:GLN:NE2	1.70	0.88
2:L:66:GLY:HA3	2:L:71:TYR:HA	1.55	0.87
2:L:44:PRO:HG2	3:H:103:TRP:CD2	2.09	0.86
1:A:69:ASN:HA	1:A:72:ILE:HG22	1.57	0.85
2:L:211:ARG:HH11	2:L:211:ARG:HB3	1.42	0.83
1:A:64:LEU:HD11	1:A:335:ALA:HB1	1.58	0.83
1:A:132:TYR:HE1	1:A:221:ARG:HG2	1.45	0.82
2:L:206:VAL:O	2:L:207:LYS:HD3	1.79	0.82
3:H:153:THR:HG23	3:H:196:ASN:HB2	1.62	0.81
1:A:71:PHE:HB3	1:A:127:ILE:HD11	1.60	0.81
3:H:147:PRO:HD2	3:H:201:ALA:HB1	1.62	0.81
2:L:190:ASN:N	2:L:190:ASN:HD22	1.79	0.80
2:L:52:ASN:HD22	2:L:53:ARG:N	1.80	0.80
2:L:182:THR:H	2:L:185:GLU:HB2	1.47	0.79
3:H:40:ARG:HB2	3:H:40:ARG:HH11	1.47	0.78
2:L:27:GLN:O	2:L:69:GLN:HG3	1.83	0.78
1:A:48:VAL:HG13	1:A:84:LEU:HD11	1.64	0.77
3:H:87:THR:HG22	3:H:90:ASP:OD2	1.85	0.77
3:H:141:LEU:HD13	3:H:141:LEU:O	1.84	0.77
1:A:337:GLN:HE21	1:A:343:ARG:HG2	1.47	0.77
3:H:109:LEU:HD12	3:H:110:THR:N	2.00	0.77
3:H:35:ASN:HD22	3:H:35:ASN:H	1.33	0.76
3:H:83:LEU:HB3	3:H:86:LEU:HD21	1.66	0.76
2:L:47:LEU:HA	2:L:58:VAL:HG21	1.69	0.75
3:H:137:THR:HA	3:H:181:VAL:O	1.87	0.75
3:H:169:VAL:HG12	3:H:170:LEU:O	1.86	0.75
3:H:40:ARG:HA	3:H:92:ALA:HB1	1.66	0.75
3:H:38:ARG:HB2	3:H:48:ILE:HD11	1.69	0.75
2:L:89:LEU:HD12	2:L:90:GLN:N	2.02	0.74
2:L:108:ARG:HG2	2:L:109:ALA:N	1.99	0.74
2:L:112:ALA:HB2	2:L:200:THR:OG1	1.86	0.74
2:L:14:SER:HB3	2:L:107:LYS:HG3	1.68	0.74
2:L:16:GLY:O	2:L:77:SER:HA	1.86	0.74
3:H:177:LEU:HD12	3:H:178:SER:N	2.03	0.73
3:H:109:LEU:HD12	3:H:110:THR:H	1.54	0.73
1:A:336:PHE:HA	1:A:339:LEU:HD23	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:116:THR:HG23	3:H:146:PHE:O	1.89	0.73
2:L:179:LEU:HD23	2:L:179:LEU:H	1.54	0.72
3:H:127:GLY:HA2	3:H:213:ARG:HH12	1.53	0.72
2:L:89:LEU:HD12	2:L:90:GLN:H	1.54	0.72
3:H:199:HIS:NE2	3:H:201:ALA:HB3	2.04	0.72
3:H:11:LEU:HD13	3:H:12:ALA:N	2.03	0.72
2:L:53:ARG:HG3	2:L:53:ARG:HH11	1.54	0.71
1:A:51:ASN:O	1:A:55:ILE:HG23	1.89	0.71
1:A:148:ASN:HD22	1:A:149:LYS:H	1.34	0.71
1:A:235:LYS:HB2	2:L:32:TYR:CZ	2.26	0.71
2:L:157:ASN:C	2:L:157:ASN:HD22	1.94	0.71
1:A:283:THR:O	1:A:287:LEU:HB2	1.91	0.70
1:A:124:LEU:HD13	1:A:279:MET:HG2	1.74	0.69
2:L:24:LYS:HG2	2:L:70:ASP:HB3	1.73	0.69
1:A:87:VAL:N	1:A:88:PRO:HD2	2.07	0.69
3:H:69:THR:OG1	3:H:82:GLN:HB3	1.91	0.69
2:L:11:MET:SD	2:L:19:VAL:HG23	2.32	0.69
1:A:52:VAL:HG13	1:A:55:ILE:HD11	1.75	0.69
1:A:52:VAL:HA	1:A:55:ILE:HG12	1.74	0.69
3:H:4:LEU:HB3	3:H:22:CYS:SG	2.33	0.69
3:H:18:VAL:HG22	3:H:86:LEU:HD11	1.74	0.69
2:L:144:ILE:HD13	2:L:145:ASN:H	1.57	0.68
1:A:127:ILE:HD12	1:A:127:ILE:H	1.56	0.68
2:L:6:GLN:HE22	2:L:101:GLY:HA2	1.57	0.68
3:H:127:GLY:HA2	3:H:213:ARG:NH1	2.08	0.68
3:H:27:TYR:CE2	3:H:98:ARG:HD2	2.28	0.68
1:A:209:TYR:O	1:A:213:VAL:HG23	1.93	0.68
2:L:136:LEU:HD21	2:L:146:VAL:HG11	1.76	0.68
3:H:97:VAL:HG12	3:H:103:TRP:HA	1.75	0.68
1:A:148:ASN:ND2	1:A:149:LYS:H	1.92	0.68
2:L:35:TRP:CD2	2:L:73:LEU:HB2	2.28	0.68
2:L:21:ILE:HB	2:L:102:THR:HG21	1.74	0.67
2:L:18:ARG:HB3	2:L:76:SER:HA	1.76	0.67
1:A:132:TYR:CE1	1:A:221:ARG:HG2	2.30	0.67
3:H:35:ASN:HD21	3:H:99:GLY:HA2	1.59	0.67
3:H:40:ARG:HB2	3:H:40:ARG:NH1	2.11	0.66
1:A:231:GLN:HE21	1:A:235:LYS:HD2	1.60	0.66
1:A:278:ILE:HG13	1:A:322:ASN:OD1	1.96	0.66
2:L:136:LEU:HD11	2:L:196:ALA:HB2	1.77	0.66
2:L:142:LYS:HA	2:L:173:TYR:CD2	2.31	0.66
2:L:108:ARG:CG	2:L:109:ALA:H	2.03	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6:GLN:HE22	3:H:96:CYS:CB	2.08	0.65
2:L:54:LEU:HD22	2:L:58:VAL:HB	1.79	0.65
1:A:267:LYS:C	1:A:267:LYS:HD3	2.17	0.65
1:A:231:GLN:C	1:A:233:ILE:H	1.97	0.65
1:A:343:ARG:HG3	1:A:344:ARG:N	2.11	0.65
3:H:214:ASP:C	3:H:216:GLY:H	2.00	0.65
2:L:95:PRO:O	2:L:97:THR:HG23	1.97	0.65
2:L:148:TRP:CE2	2:L:179:LEU:HD22	2.32	0.64
1:A:336:PHE:O	1:A:339:LEU:HG	1.97	0.64
3:H:11:LEU:HD23	3:H:147:PRO:HG3	1.80	0.64
3:H:23:LYS:HG3	3:H:78:THR:HG22	1.78	0.64
2:L:159:VAL:HG12	2:L:161:ASN:HD21	1.61	0.64
3:H:5:GLN:O	3:H:22:CYS:HA	1.97	0.64
2:L:20:THR:HG23	2:L:74:THR:OG1	1.98	0.64
2:L:24:LYS:HG2	2:L:70:ASP:CB	2.28	0.64
3:H:40:ARG:HG2	3:H:41:THR:H	1.63	0.64
1:A:71:PHE:CB	1:A:127:ILE:HD11	2.27	0.63
2:L:157:ASN:HD22	2:L:158:GLY:N	1.95	0.63
2:L:159:VAL:HG12	2:L:161:ASN:ND2	2.12	0.63
2:L:120:PRO:CG	2:L:130:ALA:HB1	2.27	0.63
1:A:235:LYS:HE3	2:L:92:ASP:O	1.99	0.63
1:A:44:VAL:O	1:A:48:VAL:HG23	1.98	0.62
1:A:153:ILE:O	1:A:157:VAL:HG23	1.98	0.62
2:L:79:ASP:HB3	2:L:82:ASP:OD2	1.98	0.62
1:A:148:ASN:HD22	1:A:148:ASN:N	1.97	0.62
2:L:2:ILE:HG12	2:L:2:ILE:O	1.97	0.62
1:A:270:LYS:O	1:A:273:LYS:HB3	2.00	0.62
1:A:69:ASN:HA	1:A:72:ILE:CG2	2.28	0.62
2:L:6:GLN:NE2	2:L:101:GLY:HA2	2.14	0.62
2:L:148:TRP:CZ2	2:L:179:LEU:HD22	2.35	0.62
3:H:35:ASN:HD22	3:H:35:ASN:N	1.96	0.62
1:A:134:ALA:O	1:A:137:SER:HB3	2.00	0.61
2:L:132:VAL:HB	2:L:179:LEU:HD21	1.81	0.61
3:H:188:TRP:CE3	3:H:189:PRO:HD3	2.35	0.61
2:L:49:TYR:CD1	2:L:50:ARG:HB2	2.34	0.61
1:A:205:ILE:O	1:A:210:VAL:HG23	1.99	0.61
3:H:133:ASN:ND2	3:H:134:SER:H	1.99	0.61
3:H:136:VAL:O	3:H:182:THR:HA	2.01	0.61
2:L:144:ILE:CD1	2:L:145:ASN:H	2.12	0.61
2:L:10:SER:O	2:L:11:MET:HB2	2.01	0.61
3:H:6:GLN:HE22	3:H:96:CYS:HB3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLN:NE2	1:A:343:ARG:HG2	2.16	0.61
3:H:56:GLY:O	3:H:58:ILE:HG13	2.00	0.61
1:A:242:VAL:HG23	3:H:32:TYR:OH	2.00	0.60
3:H:33:TYR:HA	3:H:53:PRO:HD2	1.83	0.60
2:L:59:PRO:HG2	2:L:62:PHE:CE1	2.37	0.60
3:H:34:ILE:HD11	3:H:79:ALA:HB3	1.82	0.60
3:H:6:GLN:NE2	3:H:96:CYS:HB3	2.16	0.60
3:H:40:ARG:HA	3:H:92:ALA:CB	2.30	0.60
3:H:142:VAL:O	3:H:142:VAL:HG22	2.00	0.60
1:A:231:GLN:C	1:A:233:ILE:N	2.54	0.60
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.67	0.60
2:L:44:PRO:HG2	3:H:103:TRP:CG	2.37	0.60
2:L:108:ARG:HG2	2:L:108:ARG:HH11	1.67	0.60
2:L:4:MET:HE2	2:L:23:CYS:SG	2.41	0.60
1:A:275:LEU:HA	1:A:278:ILE:HG22	1.84	0.59
1:A:124:LEU:CD1	1:A:279:MET:HG2	2.31	0.59
3:H:40:ARG:HG2	3:H:41:THR:N	2.17	0.59
2:L:47:LEU:O	2:L:55:VAL:HG23	2.01	0.59
2:L:132:VAL:HB	2:L:179:LEU:CD2	2.33	0.59
2:L:113:PRO:HA	2:L:137:ASN:O	2.03	0.59
1:A:235:LYS:O	1:A:239:ARG:HD3	2.02	0.59
1:A:283:THR:HG23	1:A:284:LEU:HD12	1.84	0.59
2:L:135:PHE:CZ	3:H:180:SER:HB3	2.38	0.59
3:H:68:ALA:HA	3:H:82:GLN:O	2.02	0.59
3:H:35:ASN:N	3:H:35:ASN:ND2	2.50	0.59
2:L:71:TYR:CD1	2:L:71:TYR:N	2.70	0.58
3:H:2:VAL:O	3:H:3:GLN:HB3	2.02	0.58
2:L:190:ASN:N	2:L:190:ASN:ND2	2.51	0.58
2:L:1:ASP:HB3	2:L:95:PRO:HD2	1.85	0.58
3:H:7:SER:HB2	3:H:107:THR:HG23	1.85	0.58
1:A:44:VAL:HG22	1:A:87:VAL:HG11	1.85	0.58
1:A:83:GLY:HA2	1:A:87:VAL:CG2	2.34	0.58
2:L:111:ALA:O	2:L:139:PHE:HA	2.04	0.58
2:L:80:TYR:CD1	2:L:81:ALA:N	2.72	0.58
2:L:6:GLN:HE21	2:L:102:THR:HG22	1.69	0.58
3:H:6:GLN:NE2	3:H:96:CYS:CB	2.67	0.58
3:H:124:LEU:HD21	3:H:141:LEU:H	1.69	0.58
1:A:339:LEU:HD12	1:A:339:LEU:C	2.25	0.57
1:A:71:PHE:O	1:A:74:SER:HB3	2.05	0.57
1:A:239:ARG:HB2	3:H:99:GLY:O	2.04	0.57
1:A:332:PHE:HA	1:A:335:ALA:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:53:ARG:HG3	2:L:53:ARG:NH1	2.19	0.57
2:L:8:PRO:O	2:L:102:THR:HB	2.04	0.57
2:L:160:LEU:HD23	2:L:160:LEU:O	2.05	0.57
3:H:138:LEU:HD12	3:H:210:ILE:HD12	1.86	0.57
3:H:166:PHE:N	3:H:166:PHE:CD1	2.71	0.57
2:L:15:LEU:CD1	2:L:106:ILE:HG21	2.34	0.57
2:L:4:MET:SD	2:L:90:GLN:HB3	2.44	0.57
3:H:71:THR:HG23	3:H:80:TYR:HB2	1.86	0.57
1:A:235:LYS:HB2	2:L:32:TYR:CE1	2.40	0.57
2:L:136:LEU:CD1	2:L:196:ALA:HB2	2.34	0.57
2:L:160:LEU:HD23	2:L:160:LEU:C	2.25	0.57
1:A:230:LEU:O	1:A:233:ILE:HD12	2.05	0.57
2:L:182:THR:HG22	2:L:183:LYS:H	1.69	0.57
1:A:52:VAL:O	1:A:55:ILE:HG12	2.05	0.57
1:A:327:CYS:O	1:A:333:ARG:HG2	2.05	0.57
2:L:52:ASN:HD22	2:L:53:ARG:H	1.49	0.57
2:L:63:ILE:N	2:L:74:THR:O	2.37	0.57
1:A:128:ALA:O	1:A:218:VAL:HG12	2.05	0.56
1:A:148:ASN:HD22	1:A:149:LYS:N	2.03	0.56
1:A:83:GLY:HA2	1:A:87:VAL:HG23	1.86	0.56
1:A:283:THR:HG23	1:A:284:LEU:CD1	2.35	0.56
1:A:337:GLN:O	1:A:343:ARG:HB2	2.05	0.56
2:L:170:ASP:OD2	2:L:172:THR:HG21	2.05	0.56
2:L:59:PRO:HG2	2:L:62:PHE:HE1	1.70	0.56
3:H:214:ASP:O	3:H:216:GLY:N	2.38	0.56
1:A:58:ILE:HD13	1:A:58:ILE:C	2.26	0.56
3:H:121:VAL:CG2	3:H:197:VAL:HG21	2.36	0.56
2:L:29:ILE:HG22	2:L:92:ASP:HB3	1.87	0.56
1:A:83:GLY:O	1:A:88:PRO:HD3	2.04	0.56
3:H:136:VAL:HG12	3:H:138:LEU:HD23	1.87	0.56
3:H:188:TRP:CH2	3:H:212:PRO:HA	2.41	0.56
1:A:81:VAL:O	1:A:85:ALA:HB3	2.06	0.56
2:L:13:ALA:O	2:L:106:ILE:HA	2.06	0.56
3:H:40:ARG:HH11	3:H:40:ARG:CB	2.18	0.56
1:A:148:ASN:ND2	1:A:148:ASN:H	2.04	0.55
2:L:120:PRO:HG2	2:L:130:ALA:HB1	1.88	0.55
2:L:142:LYS:HB2	2:L:173:TYR:CE2	2.41	0.55
3:H:116:THR:HG22	3:H:117:THR:N	2.21	0.55
1:A:58:ILE:HG23	1:A:59:ALA:H	1.70	0.55
1:A:233:ILE:HG22	1:A:234:ASP:N	2.21	0.55
1:A:141:TYR:OH	1:A:272:LEU:HD21	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:139:PHE:CE1	2:L:144:ILE:HB	2.41	0.55
3:H:67:LYS:HG3	3:H:83:LEU:CD1	2.36	0.55
1:A:121:ILE:HD13	1:A:121:ILE:O	2.06	0.55
1:A:220:SER:O	1:A:224:GLN:HG2	2.07	0.55
2:L:200:THR:HG23	2:L:201:SER:N	2.22	0.55
3:H:51:ILE:HG12	3:H:58:ILE:HG12	1.87	0.55
1:A:326:TYR:HA	1:A:330:PRO:CD	2.36	0.55
2:L:198:HIS:HD2	2:L:200:THR:HB	1.72	0.55
2:L:50:ARG:HH21	2:L:53:ARG:HH12	1.55	0.54
3:H:51:ILE:CG1	3:H:58:ILE:HG12	2.36	0.54
2:L:52:ASN:ND2	2:L:53:ARG:N	2.55	0.54
3:H:35:ASN:ND2	3:H:99:GLY:HA2	2.21	0.54
1:A:110:THR:O	1:A:110:THR:HG22	2.07	0.54
3:H:6:GLN:HG2	3:H:107:THR:OG1	2.08	0.54
1:A:240:PHE:O	1:A:242:VAL:N	2.39	0.54
3:H:138:LEU:HD23	3:H:138:LEU:N	2.23	0.54
3:H:151:THR:HB	3:H:198:ALA:HB3	1.90	0.54
2:L:38:GLN:NE2	3:H:39:GLN:NE2	2.38	0.54
3:H:110:THR:HG21	3:H:147:PRO:HB2	1.89	0.54
1:A:58:ILE:HD13	1:A:59:ALA:N	2.23	0.54
1:A:229:GLN:NE2	1:A:264:PHE:HB3	2.22	0.54
1:A:209:TYR:C	1:A:213:VAL:HG23	2.29	0.53
2:L:11:MET:CE	2:L:13:ALA:HB2	2.38	0.53
1:A:135:ILE:HD12	1:A:222:VAL:HG13	1.89	0.53
2:L:47:LEU:C	2:L:55:VAL:HG23	2.28	0.53
3:H:47:TRP:CE3	3:H:61:ASN:HB2	2.44	0.53
3:H:48:ILE:O	3:H:48:ILE:HG22	2.07	0.53
3:H:145:TYR:O	3:H:146:PHE:HB2	2.08	0.53
1:A:50:GLY:O	1:A:54:VAL:HG23	2.08	0.53
1:A:229:GLN:O	1:A:231:GLN:N	2.41	0.53
2:L:184:ASP:O	2:L:185:GLU:C	2.47	0.53
3:H:60:TYR:CE2	3:H:69:THR:HA	2.43	0.53
1:A:336:PHE:HD2	1:A:337:GLN:N	2.05	0.53
2:L:125:LEU:CD2	2:L:130:ALA:HB2	2.38	0.53
1:A:287:LEU:HD22	1:A:291:ILE:HG13	1.89	0.53
2:L:29:ILE:HG22	2:L:92:ASP:CB	2.38	0.53
3:H:36:TRP:O	3:H:48:ILE:HB	2.09	0.53
3:H:38:ARG:HD2	3:H:46:GLU:CD	2.29	0.53
1:A:54:VAL:O	1:A:58:ILE:HG22	2.08	0.53
2:L:52:ASN:HD21	2:L:53:ARG:HH11	1.57	0.53
3:H:132:THR:O	3:H:133:ASN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:137:THR:HG22	3:H:182:THR:OG1	2.09	0.53
3:H:148:GLU:OE1	3:H:149:PRO:HA	2.07	0.53
1:A:66:THR:O	1:A:70:TYR:HB2	2.09	0.53
2:L:115:VAL:HA	2:L:135:PHE:O	2.09	0.53
1:A:275:LEU:HA	1:A:278:ILE:CG2	2.38	0.52
2:L:137:ASN:HD22	2:L:174:SER:HB3	1.74	0.52
2:L:85:ILE:HG12	2:L:103:LYS:HG3	1.92	0.52
1:A:148:ASN:ND2	1:A:148:ASN:N	2.58	0.52
3:H:99:GLY:O	3:H:100:PHE:HB2	2.10	0.52
1:A:329:SER:HB2	1:A:330:PRO:HD3	1.90	0.52
1:A:234:ASP:O	1:A:237:GLU:HB2	2.09	0.52
2:L:108:ARG:HG2	2:L:108:ARG:NH1	2.25	0.52
2:L:206:VAL:HG12	2:L:207:LYS:N	2.25	0.52
1:A:139:PHE:CZ	1:A:140:LYS:HE2	2.45	0.52
2:L:125:LEU:HD23	2:L:130:ALA:HB2	1.91	0.52
2:L:209:PHE:CD1	2:L:209:PHE:C	2.82	0.52
3:H:11:LEU:HD23	3:H:147:PRO:CG	2.40	0.52
2:L:19:VAL:HG13	2:L:75:ILE:HG23	1.92	0.52
3:H:147:PRO:HD2	3:H:201:ALA:CB	2.38	0.51
1:A:82:MET:O	1:A:87:VAL:HG23	2.11	0.51
1:A:71:PHE:O	1:A:75:LEU:HD13	2.11	0.51
3:H:34:ILE:HD11	3:H:79:ALA:CB	2.39	0.51
3:H:34:ILE:HB	3:H:97:VAL:O	2.10	0.51
3:H:133:ASN:HB3	3:H:135:ALA:O	2.10	0.51
3:H:150:VAL:HG23	3:H:150:VAL:O	2.10	0.51
2:L:182:THR:HG22	2:L:183:LYS:N	2.26	0.51
3:H:144:GLY:C	3:H:174:LEU:HD12	2.31	0.51
2:L:135:PHE:CE1	3:H:180:SER:HB3	2.45	0.51
1:A:344:ARG:C	1:A:346:SER:H	2.14	0.51
2:L:61:ARG:O	2:L:75:ILE:HA	2.10	0.51
3:H:144:GLY:CA	3:H:174:LEU:HD12	2.41	0.51
3:H:4:LEU:CD1	3:H:102:TYR:HD2	2.24	0.51
3:H:11:LEU:HD13	3:H:12:ALA:H	1.75	0.51
3:H:188:TRP:CZ2	3:H:212:PRO:HA	2.46	0.51
1:A:127:ILE:HD12	1:A:127:ILE:N	2.24	0.51
1:A:146:THR:HG1	1:A:149:LYS:HB2	1.75	0.51
2:L:198:HIS:CD2	2:L:200:THR:HB	2.46	0.51
2:L:35:TRP:HB3	2:L:73:LEU:HD22	1.93	0.50
1:A:212:LEU:HD23	1:A:212:LEU:O	2.11	0.50
3:H:114:ALA:HB3	3:H:146:PHE:CZ	2.47	0.50
2:L:199:LYS:O	2:L:200:THR:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:148:GLU:OE1	3:H:148:GLU:HA	2.11	0.50
1:A:325:ILE:O	1:A:329:SER:HB2	2.12	0.50
2:L:6:GLN:HE21	2:L:102:THR:CG2	2.25	0.50
2:L:197:THR:HG22	2:L:204:PRO:HG3	1.94	0.50
1:A:267:LYS:C	1:A:269:HIS:H	2.15	0.50
1:A:88:PRO:HG2	1:A:89:PHE:H	1.77	0.50
1:A:233:ILE:CG2	1:A:234:ASP:N	2.74	0.50
2:L:19:VAL:HG22	2:L:20:THR:N	2.27	0.50
2:L:155:ARG:HG2	2:L:156:GLN:N	2.26	0.50
3:H:40:ARG:C	3:H:41:THR:O	2.49	0.50
3:H:136:VAL:HG12	3:H:137:THR:N	2.26	0.50
3:H:145:TYR:N	3:H:174:LEU:CD1	2.75	0.50
1:A:80:LEU:C	1:A:80:LEU:HD23	2.33	0.49
1:A:157:VAL:O	1:A:161:SER:HB2	2.12	0.49
2:L:4:MET:HG2	2:L:25:ALA:CB	2.42	0.49
2:L:170:ASP:OD2	2:L:172:THR:CG2	2.60	0.49
3:H:12:ALA:O	3:H:111:VAL:HA	2.12	0.49
1:A:117:VAL:HG21	1:A:286:TRP:CH2	2.46	0.49
1:A:148:ASN:ND2	1:A:149:LYS:N	2.58	0.49
2:L:49:TYR:HD1	2:L:50:ARG:HB2	1.74	0.49
3:H:168:ALA:HB2	3:H:177:LEU:HD23	1.94	0.49
3:H:48:ILE:HG23	3:H:64:PHE:CG	2.47	0.49
1:A:224:GLN:O	1:A:227:LYS:HB2	2.12	0.49
2:L:2:ILE:HG13	2:L:26:SER:OG	2.13	0.49
1:A:146:THR:OG1	1:A:148:ASN:ND2	2.46	0.49
2:L:18:ARG:CB	2:L:76:SER:HA	2.41	0.49
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.47	0.49
2:L:33:LEU:C	2:L:33:LEU:HD23	2.32	0.49
3:H:52:TYR:HD2	3:H:55:SER:HB3	1.77	0.49
3:H:136:VAL:HG23	3:H:185:SER:HB3	1.95	0.49
3:H:146:PHE:CD1	3:H:146:PHE:C	2.86	0.49
2:L:47:LEU:HA	2:L:58:VAL:CG2	2.41	0.49
2:L:139:PHE:CD2	2:L:173:TYR:O	2.66	0.49
2:L:157:ASN:C	2:L:157:ASN:ND2	2.65	0.49
1:A:52:VAL:CA	1:A:55:ILE:HG12	2.42	0.48
1:A:324:LEU:C	1:A:324:LEU:HD23	2.33	0.48
1:A:332:PHE:O	1:A:333:ARG:C	2.51	0.48
3:H:11:LEU:HD21	3:H:146:PHE:HE1	1.78	0.48
3:H:163:VAL:HG13	3:H:163:VAL:O	2.13	0.48
3:H:188:TRP:CG	3:H:189:PRO:N	2.81	0.48
2:L:108:ARG:HB3	2:L:140:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:138:LEU:HD12	3:H:210:ILE:CD1	2.42	0.48
1:A:87:VAL:N	1:A:88:PRO:CD	2.75	0.48
1:A:344:ARG:O	1:A:348:LYS:HB2	2.13	0.48
2:L:29:ILE:HD12	2:L:33:LEU:HB2	1.95	0.48
2:L:78:LEU:HD12	2:L:82:ASP:HB2	1.93	0.48
3:H:116:THR:CG2	3:H:117:THR:N	2.77	0.48
3:H:30:THR:O	3:H:31:ASP:OD1	2.31	0.48
3:H:146:PHE:CD1	3:H:147:PRO:N	2.81	0.48
1:A:329:SER:CB	1:A:330:PRO:HD3	2.44	0.48
1:A:336:PHE:CD2	1:A:337:GLN:N	2.81	0.48
1:A:58:ILE:HG23	1:A:59:ALA:N	2.29	0.48
2:L:144:ILE:HG23	2:L:145:ASN:N	2.29	0.48
3:H:47:TRP:CZ3	3:H:61:ASN:HB2	2.49	0.48
3:H:177:LEU:HD12	3:H:177:LEU:C	2.33	0.48
1:A:133:PHE:O	1:A:137:SER:HB2	2.14	0.47
2:L:140:TYR:CD1	2:L:140:TYR:C	2.88	0.47
3:H:121:VAL:HG21	3:H:197:VAL:HG21	1.96	0.47
1:A:132:TYR:O	1:A:136:THR:HG22	2.14	0.47
1:A:52:VAL:O	1:A:56:THR:HG22	2.13	0.47
1:A:112:ILE:O	1:A:116:CYS:SG	2.71	0.47
1:A:117:VAL:HG11	1:A:286:TRP:CZ3	2.49	0.47
3:H:188:TRP:O	3:H:191:GLU:O	2.33	0.47
1:A:326:TYR:C	1:A:330:PRO:HD2	2.35	0.47
3:H:4:LEU:N	3:H:4:LEU:HD12	2.30	0.47
3:H:124:LEU:HD22	3:H:140:CYS:HA	1.96	0.47
3:H:142:VAL:O	3:H:142:VAL:CG2	2.62	0.47
3:H:153:THR:OG1	3:H:154:TRP:N	2.48	0.47
1:A:238:GLY:O	3:H:32:TYR:HA	2.15	0.47
1:A:342:LEU:HB3	1:A:346:SER:CB	2.44	0.47
3:H:128:SER:HA	3:H:217:CYS:O	2.15	0.47
3:H:145:TYR:CE1	3:H:150:VAL:HG13	2.49	0.47
2:L:161:ASN:N	2:L:161:ASN:HD22	2.11	0.47
2:L:211:ARG:HH11	2:L:211:ARG:CB	2.21	0.47
3:H:67:LYS:HG3	3:H:83:LEU:HD11	1.96	0.47
2:L:19:VAL:CG1	2:L:75:ILE:HG23	2.45	0.47
2:L:70:ASP:C	2:L:71:TYR:CD1	2.88	0.47
2:L:195:GLU:HG2	2:L:206:VAL:HG22	1.96	0.47
3:H:146:PHE:CG	3:H:147:PRO:HA	2.50	0.47
3:H:199:HIS:HE2	3:H:201:ALA:HB3	1.77	0.47
2:L:19:VAL:CG2	2:L:20:THR:N	2.78	0.47
1:A:52:VAL:HG22	1:A:80:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD22	1:A:269:HIS:CE1	2.49	0.47
3:H:200:PRO:O	3:H:202:SER:N	2.48	0.47
1:A:240:PHE:O	1:A:241:HIS:C	2.52	0.46
1:A:124:LEU:HD12	1:A:215:MET:HE2	1.96	0.46
3:H:200:PRO:O	3:H:201:ALA:C	2.53	0.46
1:A:43:ILE:HG22	1:A:43:ILE:O	2.14	0.46
3:H:128:SER:HA	3:H:217:CYS:C	2.36	0.46
3:H:154:TRP:CZ3	3:H:181:VAL:HG11	2.50	0.46
3:H:155:ASN:ND2	3:H:159:LEU:HD13	2.31	0.46
2:L:136:LEU:CD2	2:L:146:VAL:HG11	2.43	0.46
3:H:160:SER:O	3:H:163:VAL:HG12	2.16	0.46
2:L:27:GLN:HB3	2:L:28:ASP:H	1.34	0.46
2:L:179:LEU:HD23	2:L:179:LEU:N	2.25	0.46
3:H:24:ALA:HB1	3:H:27:TYR:HE1	1.80	0.46
1:A:204:SER:O	1:A:208:PHE:HB3	2.16	0.46
1:A:218:VAL:O	1:A:222:VAL:HG23	2.15	0.46
2:L:59:PRO:HB2	2:L:61:ARG:NH1	2.31	0.46
3:H:39:GLN:HG3	3:H:44:GLY:O	2.15	0.46
1:A:75:LEU:HD21	1:A:124:LEU:HD21	1.97	0.46
1:A:161:SER:C	1:A:164:THR:HG22	2.35	0.46
2:L:30:ASN:N	2:L:30:ASN:HD22	2.12	0.46
1:A:82:MET:O	1:A:82:MET:HG2	2.16	0.46
1:A:117:VAL:HG12	1:A:117:VAL:O	2.16	0.46
1:A:120:SER:O	1:A:124:LEU:HD23	2.16	0.46
2:L:170:ASP:O	2:L:171:SER:C	2.54	0.46
3:H:40:ARG:HG2	3:H:41:THR:HG22	1.97	0.46
3:H:199:HIS:CD2	3:H:201:ALA:HB3	2.51	0.46
3:H:211:VAL:HG13	3:H:212:PRO:HD2	1.98	0.46
1:A:287:LEU:HB3	1:A:288:PRO:HD3	1.97	0.45
1:A:347:LEU:N	1:A:347:LEU:HD22	2.31	0.45
1:A:235:LYS:O	1:A:239:ARG:CD	2.63	0.45
2:L:86:TYR:N	2:L:86:TYR:CD1	2.84	0.45
2:L:136:LEU:HD23	2:L:175:MET:HE3	1.98	0.45
1:A:48:VAL:HG22	1:A:84:LEU:HG	1.99	0.45
1:A:48:VAL:HG12	1:A:48:VAL:O	2.17	0.45
2:L:142:LYS:CA	2:L:173:TYR:CD2	2.99	0.45
2:L:189:HIS:C	2:L:190:ASN:HD22	2.19	0.45
3:H:200:PRO:C	3:H:202:SER:N	2.66	0.45
1:A:283:THR:HG23	1:A:284:LEU:N	2.31	0.45
1:A:322:ASN:C	1:A:324:LEU:H	2.20	0.45
2:L:52:ASN:HD21	2:L:53:ARG:NH1	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:44:PRO:CG	3:H:103:TRP:CD2	2.93	0.45
2:L:91:TYR:HA	2:L:96:TYR:CD2	2.52	0.45
3:H:3:GLN:HA	3:H:102:TYR:CE2	2.51	0.45
1:A:326:TYR:HA	1:A:330:PRO:HD2	1.98	0.45
2:L:52:ASN:HD22	2:L:52:ASN:C	2.18	0.45
1:A:75:LEU:HD21	1:A:124:LEU:CD2	2.47	0.45
1:A:317:VAL:C	1:A:319:SER:H	2.21	0.45
1:A:333:ARG:HG2	1:A:333:ARG:NH1	2.31	0.45
2:L:136:LEU:N	2:L:136:LEU:HD22	2.32	0.45
1:A:79:ASP:OD1	1:A:319:SER:HA	2.17	0.45
2:L:19:VAL:HG11	2:L:104:LEU:HD11	1.99	0.45
1:A:121:ILE:HD11	1:A:212:LEU:HB2	1.98	0.44
3:H:67:LYS:HE2	3:H:90:ASP:OD1	2.17	0.44
1:A:208:PHE:O	1:A:211:PRO:HG2	2.16	0.44
1:A:212:LEU:HD23	1:A:212:LEU:C	2.37	0.44
1:A:275:LEU:CA	1:A:278:ILE:HG22	2.48	0.44
2:L:85:ILE:HG23	2:L:103:LYS:HB2	1.99	0.44
2:L:195:GLU:HG2	2:L:206:VAL:HG13	1.99	0.44
3:H:145:TYR:O	3:H:174:LEU:HD13	2.17	0.44
1:A:131:ARG:O	1:A:134:ALA:HB3	2.18	0.44
2:L:121:SER:O	2:L:122:SER:C	2.54	0.44
1:A:122:GLU:O	1:A:126:VAL:HG23	2.17	0.44
1:A:229:GLN:O	1:A:230:LEU:C	2.56	0.44
1:A:271:ALA:O	1:A:274:THR:HG22	2.18	0.44
2:L:124:GLN:HG2	2:L:129:GLY:O	2.17	0.44
1:A:287:LEU:O	1:A:291:ILE:HG13	2.18	0.44
2:L:37:GLN:O	2:L:37:GLN:HG2	2.17	0.44
3:H:128:SER:O	3:H:130:ALA:N	2.51	0.44
3:H:144:GLY:HA2	3:H:174:LEU:HD12	1.98	0.44
1:A:67:VAL:HG11	1:A:130:ASP:OD2	2.18	0.44
1:A:329:SER:HB2	1:A:330:PRO:CD	2.47	0.44
2:L:15:LEU:HD11	2:L:106:ILE:HG21	2.00	0.44
2:L:30:ASN:N	2:L:30:ASN:ND2	2.66	0.44
3:H:34:ILE:HG13	3:H:34:ILE:O	2.18	0.44
2:L:36:PHE:O	2:L:86:TYR:HA	2.18	0.44
2:L:78:LEU:CD1	2:L:82:ASP:HB2	2.47	0.44
3:H:173:ASP:O	3:H:174:LEU:CD2	2.66	0.44
1:A:287:LEU:HD22	1:A:291:ILE:CG1	2.47	0.43
2:L:91:TYR:N	2:L:91:TYR:CD1	2.86	0.43
1:A:217:PHE:HA	1:A:220:SER:HB3	1.99	0.43
1:A:231:GLN:NE2	1:A:235:LYS:HD2	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:125:ALA:HB1	3:H:126:PRO:HD2	2.00	0.43
2:L:48:ILE:HG12	2:L:54:LEU:HA	2.01	0.43
3:H:170:LEU:O	3:H:171:GLN:HB2	2.17	0.43
2:L:198:HIS:O	2:L:200:THR:HG22	2.18	0.43
3:H:6:GLN:NE2	3:H:96:CYS:HB2	2.32	0.43
3:H:133:ASN:HD22	3:H:134:SER:H	1.66	0.43
2:L:4:MET:HA	2:L:25:ALA:HA	2.01	0.43
1:A:69:ASN:CA	1:A:72:ILE:HG22	2.38	0.43
2:L:19:VAL:HG13	2:L:75:ILE:CG2	2.49	0.43
2:L:21:ILE:HD11	2:L:35:TRP:CZ3	2.54	0.43
2:L:150:ILE:O	2:L:153:SER:HB3	2.19	0.43
2:L:169:LYS:HD2	2:L:169:LYS:N	2.04	0.43
2:L:198:HIS:O	2:L:199:LYS:C	2.57	0.43
3:H:7:SER:HB2	3:H:107:THR:CG2	2.46	0.43
3:H:40:ARG:O	3:H:41:THR:O	2.37	0.43
3:H:155:ASN:O	3:H:158:SER:HB2	2.18	0.43
3:H:195:CYS:O	3:H:195:CYS:SG	2.76	0.43
1:A:336:PHE:HD2	1:A:337:GLN:H	1.65	0.43
2:L:49:TYR:CD1	2:L:49:TYR:C	2.92	0.43
3:H:4:LEU:CD1	3:H:102:TYR:CD2	3.02	0.43
2:L:151:ASP:OD2	2:L:189:HIS:ND1	2.50	0.43
2:L:212:ASN:C	2:L:214:CYS:N	2.72	0.42
1:A:289:PHE:CE2	1:A:312:ASN:OD1	2.72	0.42
2:L:152:GLY:O	2:L:153:SER:O	2.37	0.42
1:A:267:LYS:HD3	1:A:267:LYS:O	2.18	0.42
1:A:329:SER:CB	1:A:330:PRO:CD	2.97	0.42
1:A:345:SER:C	1:A:347:LEU:H	2.22	0.42
2:L:151:ASP:C	2:L:153:SER:H	2.22	0.42
2:L:161:ASN:O	3:H:169:VAL:HG21	2.18	0.42
2:L:200:THR:HG23	2:L:201:SER:H	1.84	0.42
3:H:213:ARG:C	3:H:215:CYS:H	2.21	0.42
3:H:97:VAL:CG1	3:H:103:TRP:CD2	3.03	0.42
2:L:6:GLN:O	2:L:8:PRO:O	2.38	0.42
2:L:112:ALA:CB	2:L:200:THR:HG21	2.49	0.42
2:L:120:PRO:CB	2:L:130:ALA:HB1	2.49	0.42
3:H:11:LEU:HD21	3:H:146:PHE:CE1	2.54	0.42
1:A:127:ILE:H	1:A:127:ILE:CD1	2.26	0.42
1:A:345:SER:O	1:A:347:LEU:N	2.46	0.42
1:A:133:PHE:HA	1:A:136:THR:CG2	2.50	0.42
1:A:331:ASP:O	1:A:332:PHE:C	2.58	0.42
1:A:334:ILE:HG23	1:A:338:GLU:CD	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:97:VAL:CG1	3:H:103:TRP:HA	2.48	0.42
3:H:99:GLY:O	3:H:100:PHE:CB	2.66	0.42
3:H:124:LEU:HD21	3:H:141:LEU:HB3	2.02	0.42
1:A:56:THR:HG23	1:A:57:ALA:N	2.34	0.42
1:A:275:LEU:O	1:A:279:MET:HG3	2.20	0.42
2:L:70:ASP:OD1	2:L:70:ASP:N	2.52	0.42
1:A:214:ILE:HG13	1:A:215:MET:N	2.35	0.42
1:A:222:VAL:O	1:A:224:GLN:N	2.53	0.42
1:A:216:VAL:O	1:A:216:VAL:HG12	2.20	0.41
2:L:24:LYS:CG	2:L:70:ASP:HB3	2.46	0.41
2:L:79:ASP:N	2:L:82:ASP:OD2	2.48	0.41
1:A:123:THR:HG22	1:A:127:ILE:CD1	2.50	0.41
2:L:28:ASP:OD2	2:L:28:ASP:C	2.58	0.41
2:L:163:TRP:NE1	2:L:175:MET:SD	2.93	0.41
1:A:148:ASN:HD22	1:A:148:ASN:H	1.60	0.41
1:A:281:THR:O	1:A:285:CYS:SG	2.76	0.41
1:A:337:GLN:HG2	1:A:343:ARG:CB	2.51	0.41
2:L:211:ARG:O	2:L:211:ARG:HG2	2.21	0.41
1:A:336:PHE:CA	1:A:339:LEU:HD23	2.44	0.41
2:L:140:TYR:CD1	2:L:141:PRO:N	2.88	0.41
2:L:14:SER:O	2:L:78:LEU:HD23	2.21	0.41
2:L:29:ILE:HG13	2:L:29:ILE:O	2.21	0.41
2:L:159:VAL:CG1	2:L:161:ASN:HD21	2.29	0.41
3:H:41:THR:O	3:H:42:GLY:C	2.56	0.41
1:A:57:ALA:O	1:A:61:PHE:N	2.53	0.41
3:H:4:LEU:HA	3:H:24:ALA:HA	2.02	0.41
3:H:121:VAL:HG22	3:H:197:VAL:HG21	2.01	0.41
3:H:145:TYR:N	3:H:174:LEU:HD12	2.34	0.41
1:A:146:THR:OG1	1:A:149:LYS:HB2	2.20	0.41
2:L:44:PRO:O	3:H:103:TRP:CD1	2.74	0.41
2:L:55:VAL:HG12	2:L:56:ASP:N	2.36	0.41
3:H:136:VAL:HG23	3:H:185:SER:HA	2.03	0.41
2:L:149:LYS:HG2	2:L:154:GLU:HB2	2.02	0.41
3:H:58:ILE:HG21	3:H:70:LEU:HB2	2.02	0.41
1:A:74:SER:C	1:A:76:ALA:H	2.24	0.41
2:L:103:LYS:HZ3	2:L:105:GLU:HG3	1.86	0.41
3:H:18:VAL:HG13	3:H:86:LEU:HD11	2.03	0.41
3:H:117:THR:O	3:H:145:TYR:HA	2.20	0.41
2:L:50:ARG:O	2:L:52:ASN:N	2.51	0.41
3:H:126:PRO:O	3:H:213:ARG:HG3	2.21	0.41
3:H:170:LEU:HD12	3:H:171:GLN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:184:PRO:C	3:H:186:SER:N	2.73	0.40
1:A:127:ILE:HG23	1:A:131:ARG:HG2	2.03	0.40
1:A:142:GLN:O	1:A:143:SER:O	2.38	0.40
1:A:267:LYS:C	1:A:269:HIS:N	2.74	0.40
2:L:67:SER:O	2:L:69:GLN:N	2.54	0.40
2:L:71:TYR:N	2:L:71:TYR:HD1	2.19	0.40
2:L:136:LEU:HD21	2:L:146:VAL:CG1	2.49	0.40
3:H:67:LYS:HG3	3:H:83:LEU:HD12	2.01	0.40
1:A:52:VAL:HG22	1:A:80:LEU:CD1	2.51	0.40
1:A:266:LEU:O	1:A:269:HIS:HB3	2.21	0.40
2:L:61:ARG:HG2	2:L:61:ARG:HH11	1.86	0.40
1:A:131:ARG:NH1	1:A:141:TYR:HE1	2.19	0.40
3:H:6:GLN:HE22	3:H:96:CYS:HB2	1.82	0.40
3:H:29:PHE:HZ	3:H:79:ALA:HB2	1.87	0.40
3:H:168:ALA:HA	3:H:177:LEU:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3   Torsion angles   (i)

5.3.1   Protein backbone   (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/342 (60%)	155 (76%)	36 (18%)	13 (6%)	1	9
2	L	212/214 (99%)	174 (82%)	27 (13%)	11 (5%)	2	13
3	H	215/217 (99%)	157 (73%)	45 (21%)	13 (6%)	1	10
All	All	631/773 (82%)	486 (77%)	108 (17%)	37 (6%)	1	11

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	LYS
1	A	142	GLN

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Mol	Chain	Res	Type
1	A	143	SER
1	A	241	HIS
1	A	343	ARG
2	L	2	ILE
2	L	68	GLY
2	L	153	SER
3	H	129	ALA
3	H	188	TRP
3	H	212	PRO
1	A	145	LEU
1	A	230	LEU
1	A	342	LEU
1	A	345	SER
2	L	138	ASN
3	H	41	THR
3	H	127	GLY
3	H	144	GLY
3	H	171	GLN
1	A	329	SER
1	A	333	ARG
2	L	11	MET
2	L	27	GLN
3	H	16	ALA
3	H	215	CYS
2	L	169	LYS
2	L	199	LYS
2	L	72	SER
3	H	55	SER
2	L	51	ALA
2	L	101	GLY
3	H	26	GLY
3	H	119	PRO
1	A	222	VAL
1	A	83	GLY
3	H	56	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/300 (56%)	153 (92%)	14 (8%)	11	36
2	L	191/191 (100%)	165 (86%)	26 (14%)	3	14
3	H	183/183 (100%)	155 (85%)	28 (15%)	2	11
All	All	541/674 (80%)	473 (87%)	68 (13%)	4	17

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ILE
1	A	70	TYR
1	A	72	ILE
1	A	121	ILE
1	A	124	LEU
1	A	139	PHE
1	A	142	GLN
1	A	148	ASN
1	A	237	GLU
1	A	239	ARG
1	A	287	LEU
1	A	312	ASN
1	A	333	ARG
1	A	336	PHE
2	L	11	MET
2	L	27	GLN
2	L	37	GLN
2	L	38	GLN
2	L	47	LEU
2	L	50	ARG
2	L	52	ASN
2	L	70	ASP
2	L	71	TYR
2	L	75	ILE
2	L	87	TYR
2	L	91	TYR
2	L	102	THR
2	L	104	LEU
2	L	114	THR
2	L	127	SER
2	L	140	TYR
2	L	144	ILE

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Mol	Chain	Res	Type
2	L	146	VAL
2	L	154	GLU
2	L	157	ASN
2	L	179	LEU
2	L	190	ASN
2	L	193	THR
2	L	209	PHE
2	L	211	ARG
3	H	11	LEU
3	H	20	LEU
3	H	31	ASP
3	H	33	TYR
3	H	35	ASN
3	H	51	ILE
3	H	61	ASN
3	H	71	THR
3	H	77	SER
3	H	83	LEU
3	H	97	VAL
3	H	108	THR
3	H	110	THR
3	H	124	LEU
3	H	133	ASN
3	H	138	LEU
3	H	141	LEU
3	H	146	PHE
3	H	148	GLU
3	H	153	THR
3	H	155	ASN
3	H	170	LEU
3	H	174	LEU
3	H	177	LEU
3	H	185	SER
3	H	195	CYS
3	H	206	VAL
3	H	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	148	ASN

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Mol	Chain	Res	Type
1	A	231	GLN
2	L	6	GLN
2	L	30	ASN
2	L	38	GLN
2	L	52	ASN
2	L	137	ASN
2	L	161	ASN
2	L	190	ASN
2	L	198	HIS
2	L	212	ASN
3	H	6	GLN
3	H	35	ASN
3	H	133	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	216/342 (63%)	1.41	74 (34%)	0	0	58, 192, 250, 290	0
2	L	214/214 (100%)	0.10	4 (1%)	66	65	44, 86, 138, 179	0
3	H	217/217 (100%)	0.18	7 (3%)	47	46	44, 88, 154, 232	0
All	All	647/773 (83%)	0.56	85 (13%)	3	4	44, 104, 228, 290	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	MET	8.0
1	A	89	PHE	6.6
1	A	281	THR	6.4
1	A	218	VAL	5.8
1	A	146	THR	5.5
1	A	284	LEU	5.3
1	A	68	THR	5.3
1	A	37	GLY	5.3
1	A	285	CYS	5.2
1	A	280	GLY	5.0
1	A	128	ALA	4.9
1	A	88	PRO	4.8
1	A	219	TYR	4.7
1	A	62	GLU	4.6
1	A	109	TRP	4.5
1	A	145	LEU	4.3
1	A	125	CYS	4.3
1	A	63	ARG	4.3
1	A	38	ILE	4.2
1	A	112	ILE	4.1
1	A	150	ALA	4.0
1	A	85	ALA	4.0
1	A	65	GLN	3.9

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Full wwPDB X-ray Structure Validation Report 2R4S

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Mol	Chain	Res	Type	RSRZ
1	A	127	ILE	3.9
1	A	57	ALA	3.7
1	A	69	ASN	3.7
1	A	147	LYS	3.7
1	A	116	CYS	3.7
1	A	203	SER	3.7
1	A	108	PHE	3.5
1	A	210	VAL	3.4
1	A	223	PHE	3.4
1	A	152	VAL	3.3
1	A	143	SER	3.3
1	A	242	VAL	3.3
3	H	20	LEU	3.2
1	A	76	ALA	3.2
1	A	73	THR	3.2
1	A	283	THR	3.1
1	A	130	ASP	3.1
3	H	78	THR	3.1
1	A	86	VAL	3.0
1	A	114	VAL	3.0
2	L	19	VAL	3.0
1	A	42	LEU	2.9
1	A	272	LEU	2.9
1	A	205	ILE	2.9
1	A	67	VAL	2.8
1	A	278	ILE	2.8
3	H	74	LYS	2.8
1	A	131	ARG	2.8
1	A	129	VAL	2.8
2	L	62	PHE	2.8
1	A	214	ILE	2.7
1	A	53	LEU	2.7
3	H	11	LEU	2.7
1	A	286	TRP	2.7
1	A	211	PRO	2.7
1	A	348	LYS	2.7
3	H	73	ASP	2.7
1	A	39	VAL	2.7
1	A	126	VAL	2.6
1	A	230	LEU	2.6
1	A	346	SER	2.6
1	A	118	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	75	ILE	2.6
1	A	113	ASP	2.5
1	A	72	ILE	2.5
1	A	110	THR	2.4
1	A	316	TYR	2.4
2	L	59	PRO	2.4
1	A	58	ILE	2.3
3	H	132	THR	2.3
1	A	274	THR	2.2
1	A	84	LEU	2.2
1	A	277	ILE	2.2
1	A	151	ARG	2.2
1	A	111	SER	2.2
3	H	134	SER	2.1
1	A	50	GLY	2.1
1	A	289	PHE	2.1
1	A	141	TYR	2.1
1	A	87	VAL	2.1
1	A	337	GLN	2.1
1	A	70	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.